Supporting Information

The Rise of Radicals in Bioinorganic Chemistry

Harry B. Gray

Jay R. Winkler

Contents

Table S1 – sequence alignment of class B 2dMCOs

Table S2 – sequence alignment of class C 2dMCOs

Table S1

Uniprot sequence alignment (http://www.uniprot.org/align/)

Class B, 2dMCO

Red Highlight = Tyrosine

Magenta Highlight = Tryptophan

* = complete conservation

: = conservation of amino acids with strongly similar properties

. = conservation of amino acids with weakly similar properties

```
Streptomyces griseoflavus      ---MDRRGFNRRVLLGGVAATTSLSIAPEAVSAPESAGTAAAAGAAPAGGEVRRVTMYAE 57
Streptomyces viridochromogenes ---MDRRSFNRRVLLGGATVATSLSLTSV----PEVAGAAAPARTAPAGGEVRHLKLYIE 53
Streptomyces coelicolor        ---MDRRGFNRRVLLGGAAAATSLSIAPEVAGAAPA-AKGITARTAPAGGEVRHLKMYAE 56
Streptomyces lividans          ---MDRRGFNRRVLLGGAAAATSLSIAPEVAGAAPA-AKGITARTAPAGGEVRHLKMYAE 56
Streptomyces sviceus           MGALDRRGFNRRVLLGGAAVATSLSLAP------EARSDAGPAQ-AAPGGEVRRIKLYAE 53
Streptomyces viridosporus      ------------------------------------MGPAKTAPAGGEVKRIKLYAE 21
                                                                     *  *  ****:::.:* *
Amycolatopsis sp. (ATCC 39116) ------------------------------------------MPVRAQGTTRRITMYAE 17
                                                                          .   * .::::.:* *

Streptomyces griseoflavus      RLAGGQMGYGLEKGKASIPGPLIELNEGDTLHVEFENTMDVPVSLHVHGLDYEISSDGTK 117
Streptomyces viridochromogenes KLADGQLGYGFEKGRATIPGPLIELNEGDTAHIEVENTLDVPASLHVHGLDYEITSDGTK 113
Streptomyces coelicolor        KLADGQMGYGFEKGKASVPGPLIEVNEGDTLHIEFTNTMDVRASLHVHGLDYEISSDGTA 116
Streptomyces lividans          KLADGQMGYGFEKGKASVPGPLIEVNEGDTLHIEFTNTMDVRASLHVHGLDYEISSDGTA 116
Streptomyces sviceus           RLADGQMGYGLEKGRATIPGPLIELNEGDTLHIEFENTMDVRASLHVHGLDYEVSSDGTT 113
Streptomyces viridosporus      RLGGGQMGYGLEKGKATIPGPLIELNEGDTLHIEFENTMDVPVSLHVHGLDYEISSDGTK 81
                               :*. **:***:***:*::******:***** *:*. **:** .**********::****
Amycolatopsis sp. (ATCC 39116) KISDELYGYGLAPGGATVPGPVLEMWEGDTLEIDLVNTTDRVLSLHPHGVDYDVNSDGTL 77
                               ::.    ***:  * *::***::*: **** .::. ** *   *** **:**::.****

Streptomyces griseoflavus      QNKSHVEPGGTRTYTWRTHEPGRRADGTWRAGSAGYWHYHDHVVGTEHGTGGIRNGLYGP 177
Streptomyces viridochromogenes LNRSDVEPGGTRTYTWRTHAPGRRADGTWRAGSAGYWHYHDHVVGTEHGTGGIRKGLYGP 173
Streptomyces coelicolor        MNKSDVEPGGTRTYTWRTHKPGRRDDGTWRPGSAGYWHYHDHVVGTEHGTGGIRNGLYGP 176
Streptomyces lividans          MNKSDVEPGGTRTYTWRTHKPGRRDDGTWRPGSAGYWHYHDHVVGTEHGTGGIRNGLYGP 176
Streptomyces sviceus           LNKSDVEPGGTRTYTWRTHAPGRRSDGTWRAGSAGYWHYHDHVVGTEHGTGGIRKGLYGP 173
Streptomyces viridosporus      QSRSDVEPGGTRTYTWRTHVPGRRADGTWRAGSAGYWHYHDHVVGTEHGTGGIRNGLYGP 141
                                .:*.************** **** ***** ************************:*****
Amycolatopsis sp. (ATCC 39116) MNGSAVMPGQTRRYTWRSHVGYRRADGSWAEGTAGYWHYHDHAMGTEHGTEGVLKGLYGA 137
                                . * * ** ** ****:*   ** **:*  *:*********.:****** *: :****
```

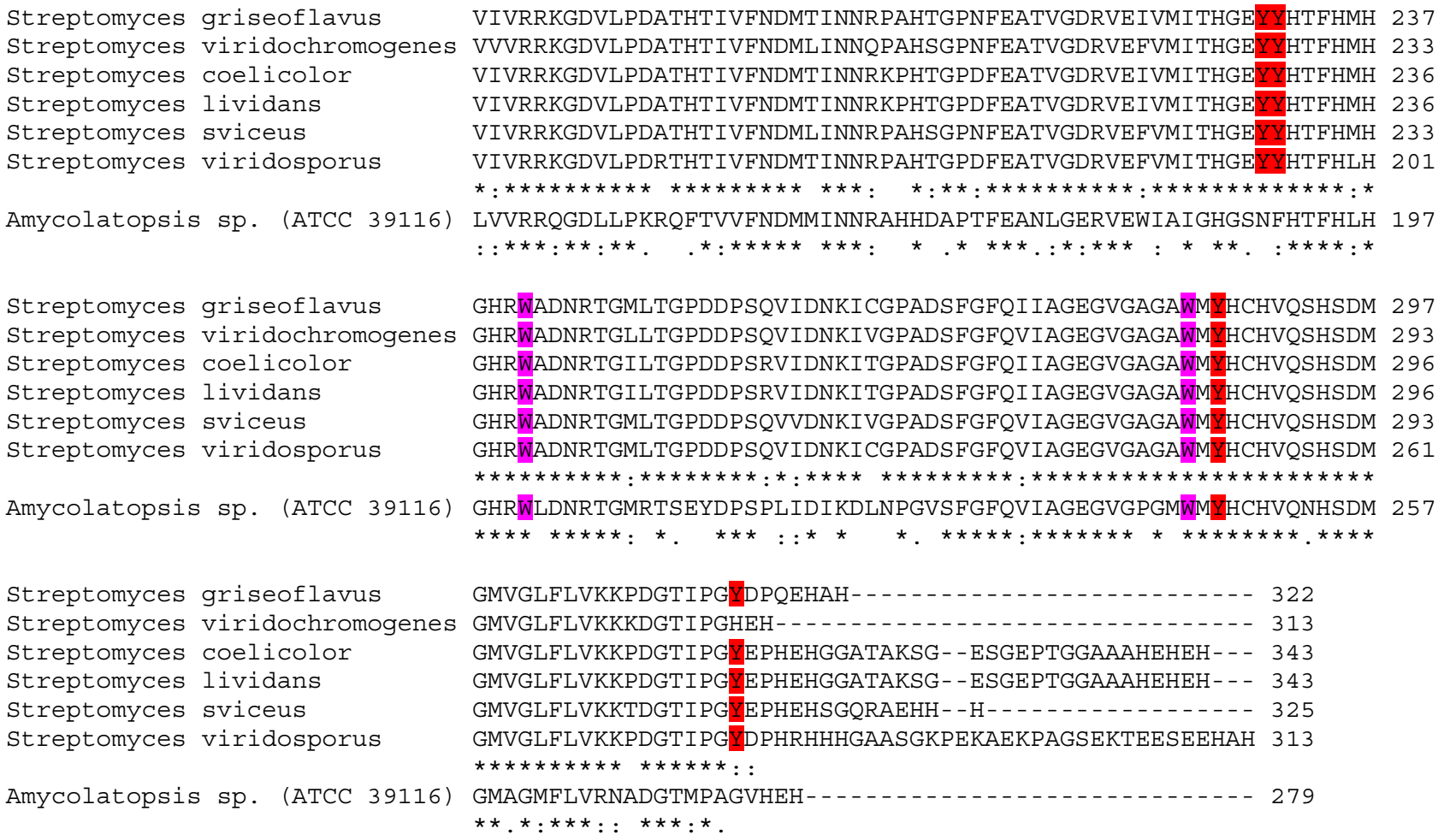
Streptomyces griseoflavus VIVRRKGDVLPDATHTIVFNDMTINNRPAHTGPNFEATVGDRVEIVMITHGEYYHTFHMH 237
Streptomyces viridochromogenes VVVRRKGDVLPDATHTIVFNDMLINNQPAHSGPNFEATVGDRVEFVMITHGEYYHTFHMH 233
Streptomyces coelicolor VIVRRKGDVLPDATHTIVFNDMTINNRKPHTGPDFEATVGDRVEIVMITHGEYYHTFHMH 236
Streptomyces lividans VIVRRKGDVLPDATHTIVFNDMTINNRKPHTGPDFEATVGDRVEIVMITHGEYYHTFHMH 236
Streptomyces sviceus VIVRRKGDVLPDATHTIVFNDMLINNRPAHSGPNFEATVGDRVEFVMITHGEYYHTFHMH 233
Streptomyces viridosporus VIVRRKGDVLPDRTHTIVFNDMTINNRPAHTGPDFEATVGDRVEFVMITHGEYYHTFHLH 201
Amycolatopsis sp. (ATCC 39116) LVVRRQGDLLPKRQFTVVFNDMMINNRAHHDAPTFEANLGERVEWIAIGHGSNFHTFHLH 197
Streptomyces griseoflavus GHRWADNRTGMLTGPDDPSQVIDNKICGPADSFGFQIIAGEGVGAGAWMYHCHVQSHSDM 297
Streptomyces viridochromogenes GHRWADNRTGLLTGPDDPSQVIDNKIVGPADSFGFQVIAGEGVGAGAWMYHCHVQSHSDM 293
Streptomyces coelicolor GHRWADNRTGILTGPDDPSRVIDNKITGPADSFGFQIIAGEGVGAGAWMYHCHVQSHSDM 296
Streptomyces lividans GHRWADNRTGILTGPDDPSRVIDNKITGPADSFGFQIIAGEGVGAGAWMYHCHVQSHSDM 296
Streptomyces sviceus GHRWADNRTGMLTGPDDPSQVVDNKIVGPADSFGFQVIAGEGVGAGAWMYHCHVQSHSDM 293
Streptomyces viridosporus GHRWADNRTGMLTGPDDPSQVIDNKICGPADSFGFQVIAGEGVGAGAWMYHCHVQSHSDM 261
Amycolatopsis sp. (ATCC 39116) GHRWLDNRTGMRTSEYDPSPLIDIKDLNPGVSFGFQVIAGEGVGPGMWMYHCHVQNHSDM 257
Streptomyces griseoflavus GMVGLFLVKKPDGTIPGYDPQEHAH---------- 322
Streptomyces viridochromogenes GMVGLFLVKKKDGTIPGHEH---------- 313
Streptomyces coelicolor GMVGLFLVKKPDGTIPGYEPHEHGGATAKSG--ESGEPTGGAAAHEHEH--- 343
Streptomyces lividans GMVGLFLVKKPDGTIPGYEPHEHGGATAKSG--ESGEPTGGAAAHEHEH--- 343
Streptomyces sviceus GMVGLFLVKKTDGTIPGYEPHEHSGQRAEHH--H---------- 325
Streptomyces viridosporus GMVGLFLVKKPDGTIPGYDPHRHHHGAASGKPEKAEKPAGSEKTEESEEHAH 313
Amycolatopsis sp. (ATCC 39116) GMAGMFLVRNADGTMPAGVHEH---------- 279

Table S2

Uniprot sequence alignment (http://www.uniprot.org/align/)

Class C, 2dMCO

Red Highlight = Tyrosine

Magenta Highlight = Tryptophan

* = complete conservation

: = conservation of amino acids with strongly similar properties

. = conservation of amino acids with weakly similar properties

```
Arthrobacter sp. (strain FB24) MPKKLSETLPSRRSMLSGAAAFAALPAFSALQPQASGGHDGHGGSGNGGGVTPPPNPGSV 60
Nitrosomonas europaea          ------------------------------------------------------------

Arthrobacter sp. (strain FB24) SGGHSGGGTGGTSPTAMTNHAGHAGFAGGSVLAERAGIDPTAILRDFDRGRTSTLPDGRT 120
Nitrosomonas europaea          ---------------MYLIYTKRTVFMKNSISL-FSSYRFTHIILMLIVLALIPLTSQAE 44
                                              :: :: *   *:    :.   * *:  :       * .

Arthrobacter sp. (strain FB24) LREWDIVAVDKDFEIAPGIIFKGWSYNGRIPGPTLWAREGDALRIHFTNAGAHPHTIHFH 180
Nitrosomonas europaea          KREFDLSIEDTRIVLVGKRDFHTFAFNGQVPAPLIHVMEGDDVTVNVTNMTTLPHTIHWH 104
                                **:*:   *. : :.    *: :::**::*.* : . *** : :..**  : *****:*

Arthrobacter sp. (strain FB24) GVHRAT---MDGTPGIGAGSIAPGQSFTYEFDATPFGTHLYHCHQSPLAPHIAKGLYGGF 237
Nitrosomonas europaea          GMLQRGTWQSDGVPHATQHAIEPGDTFTYKFKAEPAGTMWYHCHVNVNEHVTMRGMWGPL 164
                               *: :      **.*     :* **::***:*.* * **  **** .       :*::* :

Arthrobacter sp. (strain FB24) IVEPKEGRPPADD---EMVMVMNGYN----------TDGGDDNEFYSVNGLPFHFMDFPV 284
Nitrosomonas europaea          IVEPKNPLPIEKTVTKDYILMLSDWVSSWANKPGEGGIPGDVFDYYTINAKSFP-ETQPI 223
                               *****:  *  .    : ::::. :              **  ::*::*.  *     *:

Arthrobacter sp. (strain FB24) KVKQHELVRIHLINVLEYDPINSFHIHGNFFHY-YPTGTMLTPSEYTDTISQVQGQRGIL 343
Nitrosomonas europaea          RVKKGDVIRLRLIGAG--DHVHAIHTHGHISQIAFKDGFPLDKPIKGDTVLIGPGERYDV 281
                               :**: :::*::** .   * :.::* **.: :  :  *  *      **:    *:*  :

Arthrobacter sp. (strain FB24) ELRFPYPGKFMFHAHKTEFAELG------WMGFFEVS---AS------------------ 376
Nitrosomonas europaea          ILNMDNPGLWMIHDHVDTHTTNGDKPDGGIMTTIEYEEVGIDHPFYVWKDKKFVPDFYYE 341
                                *.:  ** :*:* *   .:  *       *  :* .    .

Arthrobacter sp. (strain FB24) ----------------------
Nitrosomonas europaea          ESLKKDLGMHNSKVFKGEPIEE 363
```